

Effects of Attractive correlation on Topological Flat-bands Model

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In this paper, we study the effects of attractive correlation on the topological insulator (*TI*) with topological flat-bands using an extended attractive Kane-Mele-Hubbard model (KMHM). In the KMHM, we found a quantum phase transition from *TI* to the superconductor (*SC*) state upon the increasing of the attractive Hubbard interaction U at the mean field level. This type of *SC* phase transition is different from the traditional *SC* phase transition which develops from the gapless Fermi Liquid. Cooperon-type gapped excitations exist in the *TI* side near this type of *SC* phase transition.

I. INTRODUCTION

The integer quantum Hall (IQH) effect was first observed in a two dimensional (2D) electron gas subjected to strong perpendicular magnetic field[1]. This effect provides the first example of topological states that beyond the Landau symmetry breaking paradigm. After this observation, Haldane, in 1988, proposed a model (the Haldane model) and he found a state which also has the IQH effect in this model but the realization of this state doesn't need the external magnetic field[2]. The Haldane model describe a system spinless fermions and the time reversal symmetry is broken in this model by its complex NNN hoppings. The state that Haldane found is also a topological one. The two type topological states we mentioned above that support IQH effect could be characterized by an topological invariant - TKNN number (the Chern number)[3]. Following the lesson from the Haldane model, people wonder naturally that whether the fractional quantum Hall (FQH) effect could also be realized in a model without external magnetic field. Recently, models with topologically nontrivial flat-bands (TFBs) were found to be an promising candidate to realize FQH effect without external magnetic field[5–7].

Along with the IQH and FQH states in which time-reversal symmetry breaking is required, time-reversal symmetry protected topological states of matters are also discovered in the quantized spin Hall effect (QSH)[8, 9]. People called them Z_2 topological insulator (*TI*) state. The typical model for the Z_2 topological insulator is the Kane-Mele (KM) model[9]. Recently, the correlated effects in *TI* states are studied by various groups with the Kane-Mele-Hubbard model as the starting point[11, 12].

In this paper, we investigate the effects of attractive interaction to a TFBs system using an attractive Kane-Mele-Hubbard model on the honeycomb lattice: H_{KM}^{H} . There are two important parts in H_{KM}^{H} : H_{EKM} and H_U , see Eq.(1). In the original KM model, the authors generalizes Haldane's model [2] to include spin with time reversal invariant spin-orbit interactions[9]. So the KM

model is a free model. H_{EKM} is the free limit ($U = 0$) of H_{KM}^{H} and is a general case of KM model i.e., the next-nearest-neighbor (NNN) hoppings for the spin- \uparrow and spin- \downarrow electrons are complex valued and complex conjugate to each other in H_{EKM} . So the Kane-Mele model is a special case of H_{EKM} i.e., when the complex valued NNN hoppings is purely imaginary or the Haldane phase $\hat{\phi}_{ij}$ in Eq.(2) is $\pi/2$. There are particle-hole symmetry in the half-filling original Kane-Mele model i.e., when the complex valued NNN hoppings is purely imaginary it reduce to a spin-orbit interactions[4]. So there are no particle-hole symmetry in H_{EKM} except $\hat{\phi}_{ij} = \pi/2$. If we varying the Haldane phase $\hat{\phi}_{ij}$ there exist a so called TFBs limit in H_{EKM} [5–7], see Fig.1(b).

Generally for the system with flat-bands, the kinetic energy will be quite suppressed and the interaction becomes highly relevant. In this paper, H_U in H_{KM}^{H} is treated by self consisted mean field method, at this level we find a *TI* – *SC* quantum phase transition as the Hubbard interaction strength increases beyond a critical value U_c in the H_{KM}^{H} model, see Fig.4. In this type *SC* phase transition, there is a kind of Cooperon-type excitations in the insulator side near the *SC* phase transition and the Cooperon-type excitations are gapped before its condensation [17, 18].

II. TOPOLOGICAL FLAT-BAND MODEL

The Hamiltonian that we study in this paper is H_{KM}^{H} , the attractive Kane-Mele-Hubbard model which can be writed as:

$$H_{\text{KM}}^{\text{H}} = H_{\text{EKM}} + H_U - \mu \sum_{i,\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}, \quad (1)$$

where $\sigma = \uparrow, \downarrow$ denotes the spin degree freedom, $H_U = -U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ represent the on-site Hubbard type attractive interaction, μ is the chemical potential. We call H_{EKM} the extended KM model whose Hamiltonian is

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written as:

$$H_{\text{EKM}} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} e^{i\hat{\phi}_{ij}\hat{\sigma}_z} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \quad (2)$$

$$- t'' \sum_{\langle\langle\langle i,j \rangle\rangle\rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c.$$

In H_{EKM} , the first term describes the nearest-neighbor (NN) hopping on the honeycomb lattice and its hopping strength t is set as the unit of energy in the rest of this paper. The second term describes the next-nearest-neighbor (NNN) hopping with a Haldane type complex strength $t'e^{i\hat{\phi}_{ij}}$, the phase factor in this term is spin dependended, i.e., $e^{i\hat{\phi}_{ij}} = e^{i\phi}$ for spin \uparrow electron that hopping clockwise in the fundamental plaquette as shown by the blue arrow in Fig.1(a) and $e^{i\hat{\phi}_{ij}} = e^{-i\phi}$ for spin \downarrow electron. This term recover the original spin-orbit coupling term of KM model when $\phi = \pi/2$ (so here t' cannot be regarded as the spin-orbit interaction strength). This term also reduces H_{EKM} 's full spin rotational SU(2) symmetry to a U(1) symmetry. Thus there is time reversal symmetry (TRS) but no full spin rotation symmetry in H_{EKM} . The last term represents the next-next-nearest-neighbor (NNNN) hopping with strength t'' , the energy bands of H_{EKM} could achieve a flat-bands limit with this term in it (more about this limit see below). In this paper, we consider the half-filling case of H_{KMH} i.e., the chemical potential $\mu = 0$.

The H_{EKM} model is the free limit ($U = 0$) of the H_{KMH} model. In terms of the basis vector $\Phi^\dagger(k) = [a_{k\uparrow}^\dagger, b_{k\uparrow}^\dagger, a_{k\downarrow}^\dagger, b_{k\downarrow}^\dagger]$, H_{KMH} could be expressed in a block-diagonal matrix form as: $H_{\text{EKM}} = \sum_k \Phi^\dagger(k) H_0(k) \Phi(k)$ where

$$H_0(k) = I_0 C + \begin{pmatrix} h_\uparrow \cdot \sigma & 0 \\ 0 & h_\downarrow \cdot \sigma \end{pmatrix} \quad (3)$$

with $\mathbf{h}_\uparrow = (h^x, h^y, h^z)$, $\mathbf{h}_\downarrow = (h^x, h^y, -h^z)$, I_0 is the 4×4 unit matrix and σ is the Pauli matrix that act on the A, B sublattice space of the bipartite honeycomb lattice. The three components of vector $\mathbf{h}_{\uparrow(\downarrow)} = (\text{Re } \gamma(k), -\text{Im } \gamma(k), D)$, where $\gamma(k) = \xi(k) + \xi''(k)$ with $\xi(k) = -t \sum_{i=1}^3 e^{ik \cdot \vec{a}_i}$ and $\xi''(k) = -t'' \sum_{i=1}^3 e^{ik \cdot \vec{c}_i}$, with $\vec{a}_1 = (1/2, -\sqrt{3}/2)$, $\vec{a}_2 = (1/2, \sqrt{3}/2)$, $\vec{a}_3 = (-1, 0)$.

$$C = -2t' \cos \phi_{ij} \sum_{i=1}^3 \cos[k \cdot \vec{b}_i]$$

$$D = -2t' \sin \phi_{ij} \sum_{i=1}^3 \sin[k \cdot \vec{b}_i] \quad (4)$$

with $\vec{b}_1 = (3/2, -\sqrt{3}/2)$, $\vec{b}_2 = (0, \sqrt{3})$, $\vec{b}_3 = (-3/2, -\sqrt{3}/2)$, see Fig.1(a). We set the lattice constant $a = 1$ in the rest of the paper. The energy dispersion of the H_{EKM} can be founded by diagonalize $H_0(k)$:

$$E_n(k) = C \pm \sqrt{(h^x)^2 + (h^y)^2 + (h^z)^2}. \quad (5)$$

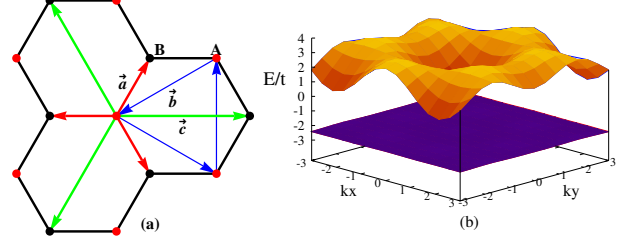


FIG. 1: (color online)(a) The honeycomb lattice consists of two sublattices: A (the red sites) and B (the black sites). The NN (red), NNN (blue) and NNNN (green) displacement vectors are denoted by \vec{a} , \vec{b} and \vec{c} respectively. The arrow in \vec{b} also denote the positive phase direction of the complex factor $e^{i\phi_{ij}}$ that company the NNN hopping. (b) The TFBs in the energy spectrum of the H_{EKM} with parameters: $t'/t = 0.6$, $t''/t = -0.58$, $\phi_{ij} = 0.4\pi$.

There are two energy bands in $E_n(k)$, both of them are doubly degenerate due to the spin degree freedom and have a flat-bands limit, i.e., with parameters: $\phi = 0.4\pi$, $t' = 0.6t$, $t'' = -0.58t$ [6]. In this limit, the lower bands of $E_n(k)$ will become flat, see Fig.1(b). The flatness ratio of the flat-bands in this limit (the ratio of the band gap over bandwidth) can reach about 50. we know that the NN and NNNN hopping energy $\xi(k)$ and $\xi''(k)$ are vanish at the two Dirac points: $(2\pi/3, 2\pi/3\sqrt{3})$ and $(2\pi/3, -2\pi/3\sqrt{3})$ in momentum space, but the NNN hopping energy $\xi'_{a(b)}(k)$ dose not, just like the spin-orbit coupling term in KM model, it will opens an energy gap at those two Dirac points. So H_{KMH} is gapped in its free limit. We denote this energy gap as $\Delta_{t'}$, it's the bulk gap of the TI state since before H_{KMH} model entering the SC phase it is in a TI phase, the magnitude of $\Delta_{t'}$ is related to t' . Thus we called $\Delta_{t'}$ the bulk gap which playing the same role as the gap of semiconductor in [17].

In H_{KMH} 's flatband limit, the Chern number for the spin up and down electron that filled the two lowest bands of $E_n(k)$ can be calculate in this way:

$$C_{\uparrow/\downarrow} = \frac{1}{4\pi} \int \mathbf{n} \cdot \left(\frac{\partial \mathbf{n}}{\partial k_x} \times \frac{\partial \mathbf{n}}{\partial k_y} \right) d^2k$$

The Chern number of spin \uparrow components electron is $C_\uparrow = 1$ with $\mathbf{n} = \mathbf{h}_\uparrow/|\mathbf{h}_\uparrow|$ and $C_\downarrow = -1$ with $\mathbf{n} = \mathbf{h}_\downarrow/|\mathbf{h}_\downarrow|$, reflecting the TRS in H_{EKM} . The spin Chern number $C_s = (C_\uparrow - C_\downarrow)/2 = 1$ reflect the QSH in the free limit of H_{KMH} model[13].

This conclusion could be further verified by the presence of edge states in the energy spectrum of H_{EKM} when it's imposed a cylinder boundary condition with zigzag edges, i.e., we set periodic boundary condition along the system's x -direction and open boundary condition along the y -direction. The numerical results are depicted in Fig.2, from which we can see that there are topologically protected edge states, which is one of the signatures of topological states of matter. So in half-filling

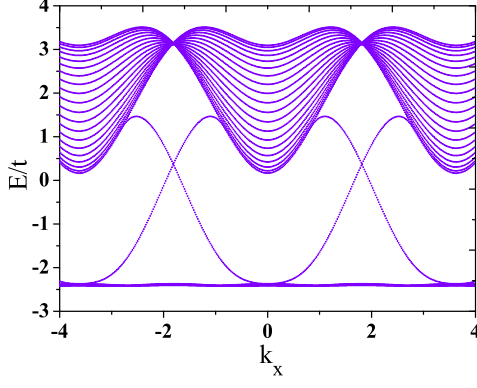


FIG. 2: (color online) The edge states of H_{EKM} in its flat-bands limit in a cylinder geometry with a zigzag edge. This is a typical edge states of TRS topological insulator which also reflecting the nontrivial topology of the flat-bands.

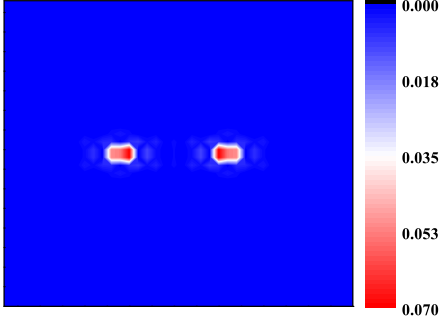


FIG. 3: (color online) The contour plots of the particle density distribution of the wave function of the zero-energy modes in coordinate space, this pair of zero-energy modes are bound to the π -fluxes. The values of particle density are indicated by color in this figure, the parameters are in H_{KMH} 's flat-bands limit.

and flat-bands limit, with the two lowest flat-bands are filled, H_{EKM} support the so called TFBs. Thus in the flat-bands limit of H_{EKM} model, it is a Z_2 TI with TFBs as a consequence of the TRS in H_{EKM} .

On the other hand, the response of TI to topological defects such as: π -fluxes has also been suggested as a probe of the nontrivial topology of the Z_2 TI [14]. Through numerical calculation, we really found that there are zero-energy modes in the energy spectrum if a pair of π -fluxes are adiabatically inserted into the H_{EKM} model in its flat-bands limit. From the particle density distribution in Fig.3, we can see that those zero-energy modes are really located around the π -fluxes in coordinate space. Those results imply that the H_{EKM} model's topological non trivial in its flat-bands limit.

III. INTERACTING FLAT-BAND MODEL

In this section, we study the effects of attractive Hubbard type interaction of H_{KMH} model in the flat-bands limit of H_{EKM} with the mean field method. In this limit, the resulting mean field phase diagram of the H_{KMH} model could be see from Fig.4(a). From Fig.4(a) we could see that the TI phase in the H_{KMH} 's free limit is unstable against an SC phase transition as the interaction strength increase beyond a finite critical value: $U_c \simeq 3.03t$.

According to the self-consistent mean field method, firstly we introduce an SC order parameter fields to decouple the Hubbard term H_U in H_{KMH} . The SC order parameter fields are defined as: $\Delta_s = \langle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rangle$. By the mean field approximation, we substitute $\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger = \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle + \delta^\dagger$ and $\hat{c}_{i\uparrow} \hat{c}_{i\downarrow} = \langle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rangle + \delta$ into the Hubbard term H_U in Eq.(1), with $\delta^\dagger = (\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger - \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \rangle)$ and $\delta = (\hat{c}_{i\uparrow} \hat{c}_{i\downarrow} - \langle \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} \rangle)$ two small quantities. We discard the second order terms of δ^\dagger and δ , then H_U could be decoupled into a bilinear form of $\hat{c}_{i\sigma}^\dagger$ and $\hat{c}_{i\sigma}$ as:

$$H_U = -U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \simeq -U \sum_i \left[\Delta_s^\dagger \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} + \Delta_s \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \right] + U N_s |\Delta_s|^2. \quad (6)$$

The honeycomb lattice's bipartite and translational invariant, so we could introduce the usual Fourier transformation to the electron creation (destruction) operator $\hat{c}_{i\sigma}^\dagger$ ($\hat{c}_{i\sigma}$) in H_{KMH} and we denote the fourier transform of $\hat{c}_{i\in A, \sigma}^\dagger$ and $\hat{c}_{i\in B, \sigma}^\dagger$ as $\hat{a}_{k\sigma}^\dagger$ and $\hat{b}_{k\sigma}^\dagger$ respectively:

$$\begin{aligned} \hat{c}_{i\in A, \sigma}^\dagger &= \frac{1}{\sqrt{N_s}} \sum_k \hat{a}_{k, \sigma}^\dagger e^{ik \cdot R_i}, \\ \hat{c}_{i\in B, \sigma}^\dagger &= \frac{1}{\sqrt{N_s}} \sum_k \hat{b}_{k, \sigma}^\dagger e^{ik \cdot R_i}. \end{aligned} \quad (7)$$

where N_s is the number of unite cells and k belong to the first Brillouin Zone of the honeycomb lattice. Now we substitute Eq.(6) and Eq.(7) into Eq.(1) we could got the momentum space form of H_{KMH} : $H_{\text{KMH}}(k)$. In the Nambu basis: $\psi^\dagger(k) = (\hat{a}_{k\uparrow}^\dagger, \hat{a}_{-k\downarrow}^\dagger, \hat{b}_{k\uparrow}^\dagger, \hat{b}_{-k\downarrow}^\dagger)$, $H_{\text{KMH}}(k)$ could be casted into a matrix form in momentum space, that's:

$$H_{\text{KMH}}(k) = \sum_k \psi^\dagger(k) h(k) \psi(k) + U N_s |\Delta_s|^2 \quad (8)$$

with the 4×4 matrix $h(k)$:

$$h(k) = \begin{pmatrix} C + D & -U\Delta_s & \gamma(k) & 0 \\ -U\Delta_s & -C - D & 0 & -\gamma(k) \\ \gamma^\dagger(k) & 0 & C - D & -U\Delta_s \\ 0 & -\gamma^\dagger(k) & -U\Delta_s & -C + D \end{pmatrix} \quad (9)$$

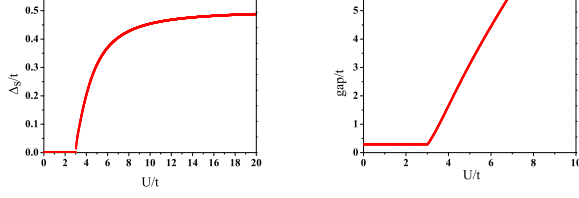


FIG. 4: (color online) (a) The mean field results of Δ_s we solve from Eq.(11) at H_{KMH} 's flat-bands limit. (b) The excitation energy gap of the SC phase as a function of the interaction strength U , this excitation gap increases with U monotonically so there is no further topological phase transition upon varying U .

where C and D are the same as in Eq.(4). The quasi-particles spectrum can be found by diagonalize the Hamiltonian(9) in the momentum space:

$$E_n(k) = \pm \sqrt{e_1 \pm 2e_2}. \quad (10)$$

where

$$e_1 = C^2 + D^2 + |\gamma(k)|^2 + (U\Delta_s)^2, \\ e_2 = \sqrt{C^2 (D^2 + |\gamma(k)|^2)}.$$

We would investigate the instability of the TI phase of H_{KMH} in the presence SC fluctuation as the interaction strength U increases by minimizing the ground state's energy $E_0 = \sum_{n,k} E_n(k)$ against the SC order parameters Δ_s , i.e., $\partial E_0 / \partial \Delta_s = 0$. Then the self-consistent mean field equation is given by:

$$1 = \frac{U}{2N_s} \sum_k \left(\frac{1}{E_1(k)} + \frac{1}{E_2(k)} \right). \quad (11)$$

where $E_1(k) = -\sqrt{e_1 + 2e_2}$ and $E_2(k) = -\sqrt{e_1 - 2e_2}$ are the two lowest filled bands in Eq.(10).

The mean field solution of the self-consistent equation Eq.(11) are plotted in Fig.4(a) from which we can see that beyond a critical value of the attractive interaction strength: $U_c \simeq 3.03t$ the TI phase of the H_{KMH} model in its flat-bands limit become unstable against a SC phase transition.

The quasi-particles excitation gap in the SC phase increases with U monotonically, see Fig.4(b). This mean that there is no gap closing and no further topological phase transition upon varying U .

Fig.5 and Fig.6 is the mean field results of the SC order parameter Δ_s we obtained from solving Eq.(11) and the excitation gap of SC phase over a range of t' and U with the other parameters are fixed in the flat-bands limit. Note that in the presence of the bulk gap $\Delta_{t'}$ the order parameter Δ_s and the excitation gap of SC phase are not the same like in the traditional SC phase transition[17]. From Fig.5 we could infer that the critical

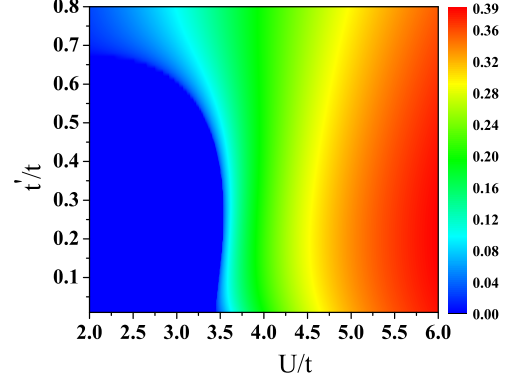


FIG. 5: (color online) The mean field results of the SC order parameter Δ_s we solve from Eq.(11) over a range of U and t' , Other parameters are in the flat-bands limit.

interaction strength U_c which separate the TI and SC phase increases nearly linearly with t' .

As a consequence of TRS in H_{KMH} , the Chern number will be zero and we verified this by a numerical calculation. We calculate the Chern number of the two lowest bands of $h(k)$ is $h(k)$ [15, 16], the numerical results show that the total Chern number $C = 0$ in the SC phase at $U = 3.03$ with $\Delta_s = 0.0147$ while the other parameters in the flat-bands limit. This mean that the SC phase transition destroy the TFBs. The topological property of this SC state can also be see from its edge excitations, so we also calculate the energy bands of H_{KMH} in a cylinder geometry. The numerical results are depicted in Fig.7 from which we can see that the edge states are gapped when the SC order is developed in H_{KMH} . So beyond the critical interaction strength U_c , H_{KMH} entering a topological trivial SC phase. On the other hand, we found a pair finite-energy bound state in the energy spectrum if a pair of π -fluxes are inserted into the SC phase with periodic boundary condition in both x and y direction, see Fig.8, comparing with the π -flux-induced zero-energy modes in Fig.3 in the TI phase, show that the SC phase is topological trivial. This finite energy bound states and the gapped edge states in Fig.7 verified that the H_{KMH} model will loss its topology properties upon entering this s-wave SC phase as the attractive interaction strength increasing.

So the SC phase in H_{KMH} develops from a fully gapped TI state. This kind of SC phase transition is different from the traditional SC phase transition which develops from a Fermi liquid in which the low energy excitations are gapless. If a SC order is develops from an fully gapped state, in our case an TI state, there will be an kind of gapped excitations, the so called Cooperon, in the insulator side of this SC phase transition[17, 18]. This type of SC phase transition's mechanism could be understand in this way. There is a competition between the SC pairing gap Δ_s and the topological energy gap $\Delta_{t'}$ upon

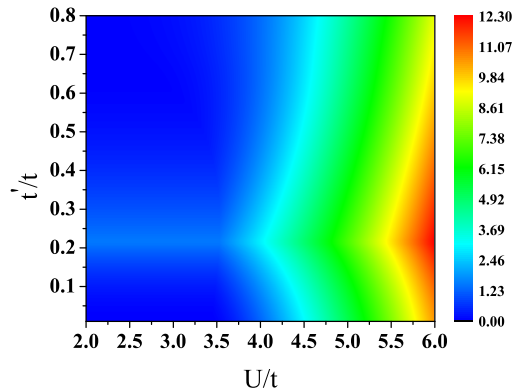


FIG. 6: (color online) The mean field results of the excitation energy gap in the SC phase over a range of U and t' while other parameters are in the flat-bands limit.

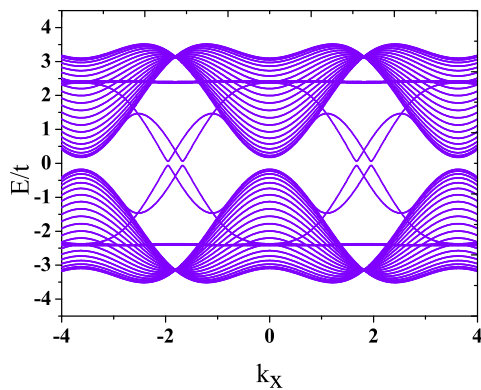


FIG. 7: (color online) Energy bands of H_{KMH} in its SC phase in a cylinder geometry with “zigzag” boundary. The SC phase is at $U = 3.91$ with $\Delta_s = 0.016t$, the other parameters are in the flat-bands limit.

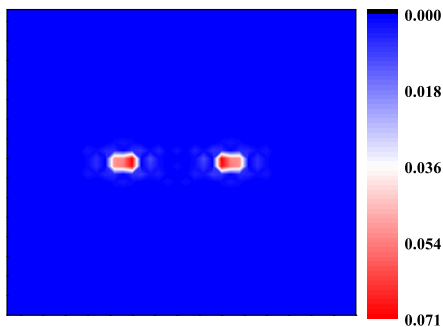


FIG. 8: (color online) The contour plots of the particle density distribution of the finite-energy bound states in the coordinate space. We can see that the finite-energy states are bound to the π -fluxes. The values of particle density are indicated by color. H_{KMH} 's in its SC phase and flat-bands limit.

the varying of interaction strength U . If the topological energy gap $\Delta_{t'}$ is large enough, the Cooperon excitations will have an energy gap and will not condense, so the SC order parameter is vanishingly small. On the other hand, if $\Delta_{t'}$ is very small or the SC energy gap is large enough (at large U), the Cooperon excitations will become gapless and condensed, their condensation will lead to the SC phase transition at last.

IV. CONCLUSION

In this paper, we study the influence of attractive correlation on TI using the H_{KMH} model via a self-consistent mean field method. In the mean field level, we found a $TI - SC$ phase transition upon increasing the attractive interaction strength U in this model. The mechanism leading to this SC phase transition is different from the traditional ones. There is a competition between the topological energy gap $\Delta_{t'}$ and the SC energy gap before the SC phase transition. This competition is reflected in the gapped Cooperon excitation, when the SC pairing gap is larger than $\Delta_{t'}$, the Cooperon excitation will condense and the SC phase transition occurs in the system eventually. We think those results may help in better understanding the quantum exotic states in the correlated topological insulator and the pseudogap state in the high T_C cuprate superconductor[19].

Acknowledgments. we thank professor Su-Peng Kou for his many helpful advices. This research is supported by National Basic Research Program of China (973 Program) under the grant No. 2011CB921803, 2012CB921704 and NFSC Grant No.11174035.

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